

Citric acid
77-92-9 | DTXSID3020332

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $1.88\text{e-}12 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

Global applicability domain: Outside

Local applicability domain index: $2.32\text{e-}01$

Confidence level: $7.69\text{e-}01$

Nearest Neighbors from the Training Set

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Dimethyl succinate

Measured: $1.40\text{e-}12$

Predicted: $1.93\text{e-}12$

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Dimethyl glutarate

Measured: $3.30\text{e-}12$

Predicted: $3.76\text{e-}12$

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Dimethyl adipate

Measured: $8.40\text{e-}12$

Predicted: $6.84\text{e-}12$

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Peroxyacetyl nitrate

Measured: $1.00\text{e-}13$

Predicted: $9.98\text{e-}14$

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Methyl 2-hydroxypropanoate

Measured: $2.80\text{e-}12$

Predicted: $3.16\text{e-}12$